1/03/06

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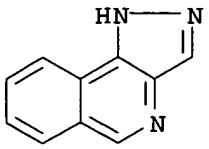
=> s l2
L3 10 L2

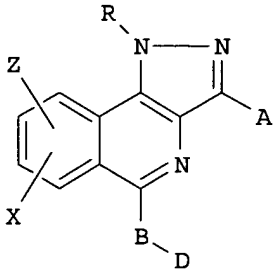
=> d abs fbib hitstr 1-10

L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
AB Theor. calcns. at semi-empirical AM1 and d. functional B3LYP/6-31G* levels were carried out on 52 NH-indazoles. Although in most cases the 1H-tautomer is the most stable, we found several indazoles for which the 2H-tautomer is more stable than the 1H-tautomer. The differences in energy between the 1H- and 2H-tautomers were interpreted in terms of substituent effects with the use of a Free-Wilson (presence-absence) matrix.
AN 2005:674931 CAPLUS
DN 143:266493
TI Theoretical estimation of the annular tautomerism of indazoles
AU Alkorta, Ibon; Elguero, Jose
CS Instituto de Quimica Medica, CSIC, Madrid, E-28006, Spain
SO Journal of Physical Organic Chemistry (2005), 18(8), 719-724
CODEN: JPOCEE; ISSN: 0894-3230
PB John Wiley & Sons Ltd.
DT Journal
LA English
IT **42318-56-9**, 1H-Pyrazolo[4,3-c]isoquinoline
RL: PRP (Properties)
(1H tautomer; theor. estimation of the annular tautomerism of indazoles)
RN 42318-56-9 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline (9CI) (CA INDEX NAME)

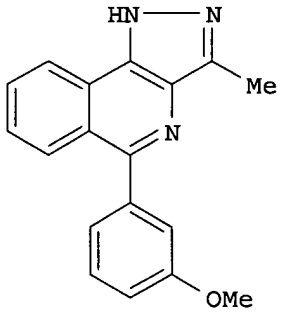


RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I



II

AB Novel pyrazoloisoquinoline derivs. I, useful as kinase inhibitors, are disclosed [wherein: A = (un)substituted alkyl, OH or derivs., SH or derivs., CO2H or derivs., NH2 or derivs., cyano, (un)substituted heteroaryl, cycloalkyl, or heterocyclyl; B = bond, (un)substituted CH:CH, C.tplbond.C, O(CH2)1-4, O, S, CO, (un)substituted NH, NHCO, CONH, NHSO2, SO2NH, NHCONH, or C1-4 alkylene; D = (un)substituted alkyl, heteroaryl, heterocyclyl, aryl, or cycloalkyl; or BD = H, halo, fluoroalkoxy, (un)substituted alkyl; R = H, alkyl, (un)substituted arylalkyl; X, Z = H, alkyl, OH, alkoxy, halo, fluoroalkyl, CO2H or derivs., NH2 or derivs., cyano, SH or derivs., (un)substituted heterocyclyl or cycloalkyl; with provisos]. I are suitable for producing pharmaceuticals for the prophylaxis and therapy of diseases whose course involves an increased activity of NIK. Approx. 75 examples were prepared, and these plus addnl. compds. are individually claimed. For instance, 3-methoxybenzoic acid was condensed with 3-methyl-5-phenyl-1H-pyrazol-4-ylamine using HOBT and DIPC, and the resultant benzamide derivative was cyclized by treatment with P2O5 and POCl3 in xylene at 160°, to give title compound II. In a test for inhibition of release of IL1β, TNFα, and IL6 in LPS-stimulated heparinized whole human blood, II had IC50 values of 1.3, 1.2, and 7 μM, resp.

AN 2005:120930 CAPLUS
DN 142:219282
TI Pyrazoloisoquinoline derivatives as kinase inhibitors, and their preparation, pharmaceutical compositions, and use in the treatment of diseases involving increased NIK activity.
IN Majid, Tahir N.; Hopkins, Corey; Pedgrift, Brian L.; Collar, Nicola; Wirtz-Brugger, Friederike; Merrill, Jean
PA Aventis Pharmaceuticals Inc., USA
SO PCT Int. Appl., 94 pp.
CODEN: PIXXD2
DT Patent

LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005012301	A1	20050210	WO 2003-US21144	20030703

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

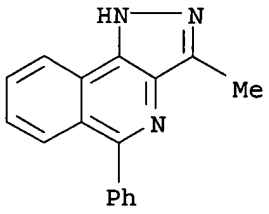
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

WO 2003-US21144 20030703

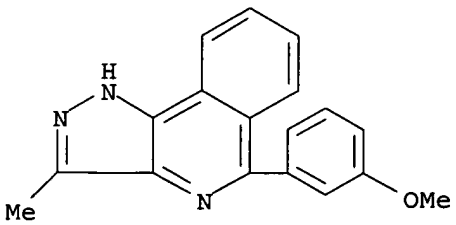
OS MARPAT 142:219282

IT **112884-48-7P**, 3-Methyl-5-phenyl-1H-pyrazolo[4,3-c]isoquinoline **645417-68-1P**, 5-(3-Methoxyphenyl)-3-methyl-1H-pyrazolo[4,3-c]isoquinoline **645417-70-5P**, 5-(2-Methoxyphenyl)-3-methyl-1H-pyrazolo[4,3-c]isoquinoline **645417-71-6P**, 5-(2,3-Dimethoxyphenyl)-3-methyl-1H-pyrazolo[4,3-c]isoquinoline **645417-75-0P**, 5-(3,5-Dimethoxyphenyl)-3-methyl-1H-pyrazolo[4,3-c]isoquinoline **645417-93-2P**, 5-Phenyl-1H-pyrazolo[4,3-c]isoquinoline-3-carboxylic acid **645417-94-3P**, Methyl 5-phenyl-1H-pyrazolo[4,3-c]isoquinoline-3-carboxylate
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrazoloisoquinoline derivs. as NIK inhibitors)

RN 112884-48-7 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-methyl-5-phenyl- (9CI) (CA INDEX NAME)



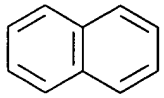
RN 645417-68-1 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 5-(3-methoxyphenyl)-3-methyl- (9CI) (CA INDEX NAME)

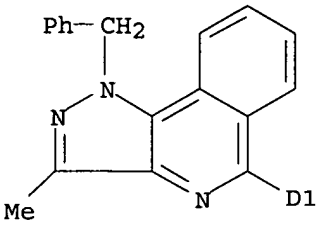


RN 645417-70-5 CAPLUS

1/03/06

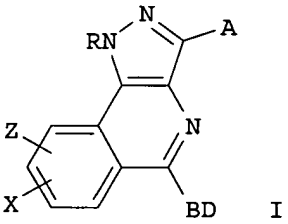
RN 843613-16-1 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-methyl-5-(naphthalenyl)-1-(phenylmethyl)- (9CI) (CA INDEX NAME)





RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
GI



I

AB Title compds. [I; A = (substituted) alkyl, heteroaryl, heterocyclyl; B = bond, C:CR1, C.tplbond.C, O(CH2)a, O, S, CO, NR2, NR2CO, (substituted) alkylene, etc.; R1 = H, alkyl, aryl, etc.; R2 = alkyl, OH, alkoxy, halo, etc.; a = 1-4; D = (substituted) alkyl, heteroaryl, heterocyclyl, aryl, cycloalkyl; BD = H, halo, fluoroalkyl, fluoroalkoxy, etc.; R = H, alkyl, (substituted) aralkyl; X, Z = H, alkyl, OH, alkoxy, halo, fluoroalkyl, CO2R1, N(R1)2, cyano, SR1, SOR1, SO2R1, (substituted) heterocyclyl, cycloalkyl, etc.; with provisos], were prepared Thus, hydroxybenzotriazole, diisopropyl carbodiimide, benzoic acid, and 3,5-diphenyl-1H-pyrazol-4-ylamine were stirred 12 h in MeCN to give a residue which was heated with P2O5 and POCl3 in xylene at 150° for 4 h followed by stirring at room temperature for 12 h to give 3,5-diphenyl-1H-pyrazolo[4,3-c]isoquinoline. The latter inhibited TNFα release in LPS-stimulated human peripheral blood lymphocytes with IC50 = 1.9 nM.
AN 2005:34602 CAPLUS
DN 142:134600
TI Preparation of pyrazoloisoquinolines as NFκB-inducing kinase (NIK) inhibitors

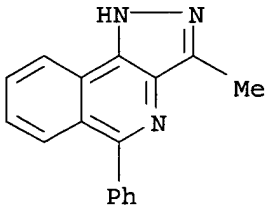
10613588

1/03/06

IN Majid, Tahir Nadeem; Hopkins, Corey; Pedgrift, Brian Leslie; Collar, Nicola; Wirtz-Brugger, Friederike; Merrill, Jean
PA Aventis Pharmaceuticals Inc., USA
SO U.S. Pat. Appl. Publ., 41 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2005009859	A1	20050113	US 2003-613588	20030703
			US 2003-613588	20030703

OS MARPAT 142:134600
IT **112884-48-7P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(claimed compound; preparation of pyrazoloisoquinolines as NFκB-inducing kinase inhibitors)
RN 112884-48-7 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-methyl-5-phenyl- (9CI) (CA INDEX NAME)



IT **112884-54-5P 112884-56-7P 824968-16-3P**
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824968-23-2P 824968-24-3P 824968-25-4P
824968-26-5P 824968-27-6P 824968-28-7P
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824968-71-0P 824968-72-1P 824968-73-2P
824968-74-3P 824968-75-4P 824968-76-5P
824968-77-6P 824968-78-7P 824968-79-8P
824968-80-1P 824968-81-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of pyrazoloisoquinolines as NFκB-inducing kinase inhibitors)

LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004005287	A1	20040115	WO 2003-EP6500	20030620
	WO 2004005287	C2	20040304		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
				DE 2002-10229762 A	20020703
	DE 10229762	A1	20040122	DE 2002-10229762	20020703
	CA 2490571	AA	20040115	CA 2003-2490571	20030620
				DE 2002-10229762 A	20020703
				WO 2003-EP6500 W	20030620
	EP 1519934	A1	20050406	EP 2003-762498	20030620
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
				DE 2002-10229762 A	20020703
				WO 2003-EP6500 W	20030620
	BR 2003012424	A	20050426	BR 2003-12424	20030620
				DE 2002-10229762 A	20020703
				WO 2003-EP6500 W	20030620
	US 2004097541	A1	20040520	US 2003-613482	20030703
	US 6841556	B2	20050111		
				DE 2002-10229762 A	20020703
				US 2002-423954P P	20021105

OS MARPAT 140:94041

IT **645417-67-0P 645417-68-1P 645417-69-2P**
645417-70-5P 645417-71-6P 645417-72-7P
645417-73-8P 645417-74-9P 645417-75-0P
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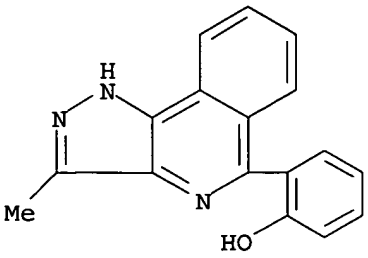
645417-79-4P 645417-80-7P 645417-81-8P
645417-82-9P 645417-83-0P 645417-84-1P
645417-85-2P 645417-86-3P 645417-87-4P
645417-88-5P 645417-89-6P 645417-90-9P
645417-91-0P 645417-92-1P 645417-93-2P
645417-94-3P 645417-95-4P 645417-96-5P
645417-97-6P 645417-98-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of pyrazoloisoquinolines as NIK inhibitors)

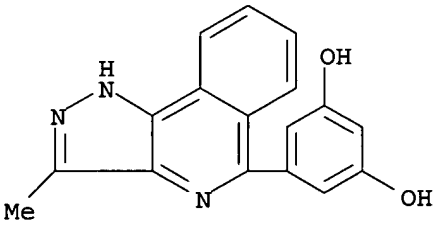
RN 645417-67-0 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 3,5-diphenyl- (9CI) (CA INDEX NAME)

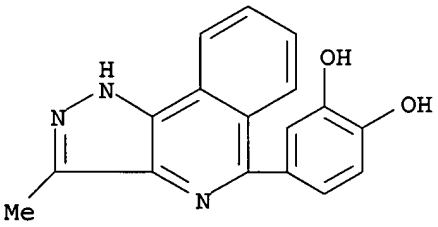
NAME)



RN 645417-97-6 CAPLUS
CN 1,3-Benzenediol, 5-(3-methyl-1H-pyrazolo[4,3-c]isoquinolin-5-yl)- (9CI) (CA INDEX NAME)



RN 645417-98-7 CAPLUS
CN 1,2-Benzenediol, 4-(3-methyl-1H-pyrazolo[4,3-c]isoquinolin-5-yl)- (9CI) (CA INDEX NAME)

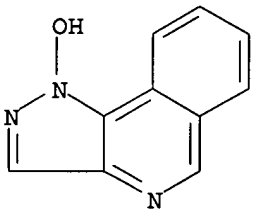


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
AB Addition-elimination reactions involving a nucleophile and a remote leaving group [SHN(AE)tele] are well-known under basic conditions, especially amongst electron-poor six-membered heterocycles, but are less commonly encountered for five-membered heterocycles and are rare under acidic conditions. Concentrated HCl converts 1-hydroxy-1H-pyrazolo[3,4-c] isoquinoline and 1-hydroxy-1H-pyrazolo[3,4-c]quinoline into 3-chloro-1H-pyrazolo[3,4-c]isoquinoline and 3-chloro-1H-pyrazolo[3,4-c]quinoline, resp. However, apparently neither the isomeric 1-hydroxy-1H-pyrazolo[4,3-c](iso)-quinolines nor the parent 1-hydroxypyrazole undergo this reaction. Addnl., all these systems are refractory under basic conditions. We present a plausible mechanism for the reaction, involving the 3-addition of Cl- to the diprotonated heterocycle, followed by the elimination of water.

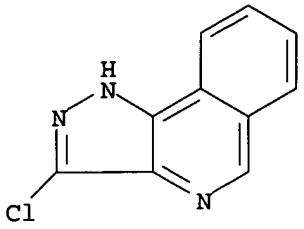
Calcns. of the initial transition states and intermediates, using optimization at B3LYP/6-311+G(d,p), including thermochem. [HF/6-31+G(d)], and single-point Poisson-Boltzmann self-consistent reaction field determination of the free energy of solvation (Jaguar Poisson-Boltzmann self-consistent reaction field), support this mechanism and reproduce the observed order of reactivity, the addition step being 2-4 kcal less favorable for the isomeric 1-hydroxy-1H-pyrazolo[4,3-c](iso)quinolines and provide a rationalization for the role of strong acid.

AN 2003:353023 CAPLUS
DN 139:307390
TI Action of HCl on 3-hydroxypyrazolo(iso)quinolines to give 1-chloropyrazoles: evidence for an addition-elimination mechanism by ab initio calculations in gas phase and water
AU Greenwood, Jeremy R.; Begtrup, Mikael
CS Department of Medicinal Chemistry, Royal Danish School of Pharmacy, Copenhagen, Den.
SO Theoretical Chemistry Accounts (2003), 109(4), 200-205
CODEN: TCACFW; ISSN: 1432-881X
PB Springer-Verlag
DT Journal
LA English
IT **610272-18-9**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(ab initio study of reaction of hydrogen chloride with 3-hydroxypyrazolo(iso)quinolines to give 1-chloropyrazoles)
RN 610272-18-9 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-hydroxy-, conjugate monoacid (9CI) (CA INDEX NAME)



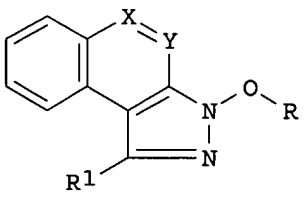
● H^+

IT **610272-29-2**
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)
(ab initio study of reaction of hydrogen chloride with 3-hydroxypyrazolo(iso)quinolines to give 1-chloropyrazoles)
RN 610272-29-2 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 3-chloro-, conjugate monoacid (9CI) (CA INDEX NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
GI



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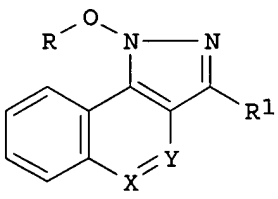
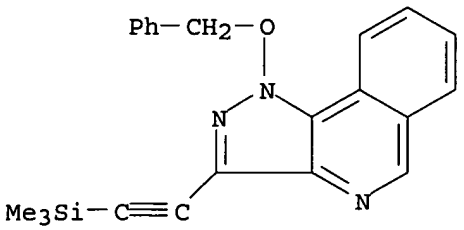


II

AB Regioselective bromination and iodination of pyrazoloquinolines and pyrazoloisoquinolines I and II (R = benzyl, R1 = H, X = N, Y = CH; R = benzyl, R1 = H, X = CH, Y = N) to form the corresponding halopyrazoles I and II (R1 = Br, I) was discussed. Reactivity differences between I (R = benzyl, R1 = H, X = N, Y = CH), I (R = benzyl, R1 = H, X = CH, Y = N) and II (R = benzyl, R1 = H, X = CH, Y = N), and the failure of II (R = benzyl, R1 = H, X = N, Y = CH) to give the expected halopyrazoles, were explained using calculated relative energies of bromination, and inspection of frontier MOs. Utility of the prepared halides was demonstrated by a series of palladium-catalyzed cross-coupling reactions.

AN 2001:246490 CAPLUS
DN 135:122430
TI Halogenation of pyrazoloquinolines and pyrazoloisoquinolines. Theoretical analysis of the regioreactivity and cross-coupling of 3-halogen derivatives
AU Pawlas, Jan; Greenwood, Jeremy; Vedso, Per; Liljefors, Tommy; Jakobsen, Palle; Huusfeldt, Per Olaf; Begtrup, Mikael
CS Department of Medicinal Chemistry, The Royal Danish School of Pharmacy, Copenhagen, DK-2100, Den.
SO Journal of the Chemical Society, Perkin Transactions 1 (2001), (8), 861-866
CODEN: JCSPCE; ISSN: 1472-7781
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 135:122430



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

AB 1-Hydroxypyrazolo[3,4-c]quinoline (I), 1-hydroxypyrazolo[4,3-c]quinoline (II), 1-hydroxypyrazolo[3,4-c]isoquinoline (III), and 1-hydroxypyrazolo[4,3-c]isoquinoline (IV) were prepared from 1-benzyloxypyrazole, establishing the pyridine B-ring in the terminal step. The pyridine ring of the 1-benzyloxy derivative of pyrazoloquinolines II and I was formed via cyclization of a formyl group at C-4 or C-5 and an amino group of a 2-aminophenyl substituent at C-5 or C-4 in 1-benzyloxypyrazole. The pyridine ring of 1-benzyloxy derivs. of pyrazoloisoquinolines III and IV was created via cyclization of a formyl group in a 2-formylphenyl substituent at C-4 or C-5 with an iminophosphorane group installed at C-5 or C-4 of 1-benzyloxypyrazole by lithiation followed by reaction with tosyl azide and then with tributylphoshine utilizing the Staudinger/aza-Wittig protocol. The 2-aminophenyl and the 2-formylphenyl substituent were introduced at C-5 or C-4 by regioselective metalation followed by transmetalation to the pyrazolylzinc halide and subsequent palladium-catalyzed cross-coupling with 2-iodoaniline or 2-bromobenzaldehyde. The order of reactions and use of protecting groups in the individual sequences have been optimized. The 1-benzyloxy-substituted pyrazoloquinolines and isoquinolines thus obtained were debenzylated by strong acid to the corresponding 1-hydroxy-substituted pyrazoloquinolines and isoquinolines I-IV.

AN 2000:847300 CAPLUS
DN 134:147535

TI Synthesis of 1-hydroxy-substituted pyrazolo[3,4-c]- and pyrazolo[4,3-c]quinolines and -isoquinolines from 4- and 5-aryl-Substituted 1-benzyloxypyrazoles

AU Pawlas, Jan; Vedso, Per; Jakobsen, Palle; Huusfeldt, Per Olaf; Begtrup, Mikael

CS Department of Medicinal Chemistry, The Royal Danish School of Pharmacy, Copenhagen, DK-2100, Den.

SO Journal of Organic Chemistry (2000), 65(26), 9001-9006
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

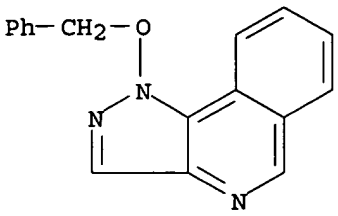
LA English

OS CASREACT 134:147535

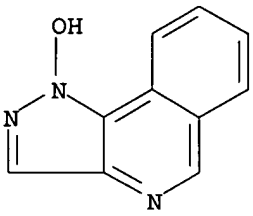
IT **323582-69-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxy pyrazoloquinolines and -isoquinolines via cyclization of arylbenzyloxypyrazoles)

RN 323582-69-0 CAPLUS

CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-(phenylmethoxy)- (9CI) (CA INDEX NAME)



IT **323583-17-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of hydroxy pyrazoloquinolines and -isoquinolines via cyclization of arylbenzyloxypyrazoles)
RN 323583-17-1 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-hydroxy- (9CI) (CA INDEX NAME)



RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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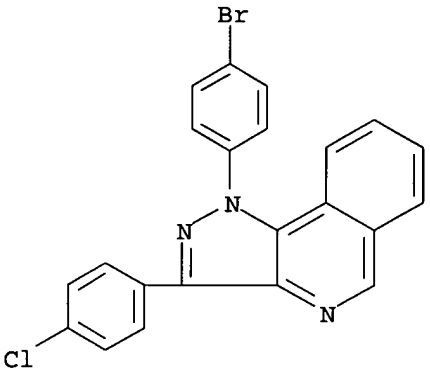
GI

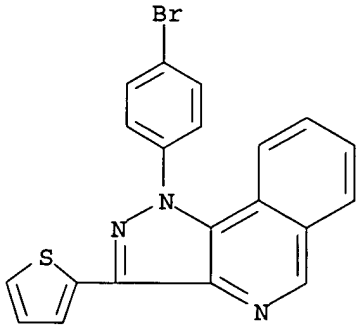
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The tetrafluoroborate salts of triazoloquinolinium cation I, triazolo[1,5-b]isoquinolinium cation II, and [1,2,3]triazolo[1,5-a]pyrazinium cation III undergo valence bond isomerization when heated in either trifluoroacetic acid or in o-dichlorobenzene to ring-opened reactive intermediates which can participate in electrophilic substitution as nitrenium cations to yield pyrazole- and indazole-fused new heterocycles, pseudoelectrocyclization of nitrenium intermediates onto electron-deficient rings, or as carbenium cations in nucleophilic addition reactions. E.g., the tetrafluoroborate of II cyclized in o-dichlorobenzene at 190° to give the indazolylisoquinoline IV in 83% yield, while cyclization of II in CF3CO2H at reflux gave arylpyrazoloisoquinoline V in 85% yield. Comparison of these and some recent results reveals that this ring opening of fused [1,2,3]triazolium salts is a general phenomenon and is closely related to the well-known retro-electrocyclizations (called "1,5-dipolar cyclizations") of neutral fused [1,2,3]triazoles and tetrazoles.
AN 1999:392479 CAPLUS
DN 131:157733
TI Valence Bond Isomerization of Fused [1,2,3]Triazolium Salts with Bridgehead Nitrogen Atom. Fused Azolium Salts. 19
AU Beres, Mariann; Hajos, Gyoergy; Riedl, Zsuzsanna; Soos, Tibor; Timari,

Geza; Messmer, Andras
CS Chemical Research Center Institute of Chemistry, Hungarian Academy of Sciences, Budapest, H-1525, Hung.
SO Journal of Organic Chemistry (1999), 64(15), 5499-5503
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:157733
IT **237417-80-0P 237417-84-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fused pyrazole and indazole heterocycles by valence bond isomerization ring cleavage and regioselective intramol. cyclization reactions of fused triazolium salts)
RN 237417-80-0 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-(4-bromophenyl)-3-(4-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 237417-84-4 CAPLUS
CN 1H-Pyrazolo[4,3-c]isoquinoline, 1-(4-bromophenyl)-3-(2-thienyl)- (9CI) (CA INDEX NAME)



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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